

Strange kinetics: conflict between density and trajectory description

M. Bologna

*Center for Nonlinear Science, University of North
Texas, P.O. Box 311427, Denton, Texas 76203-5370, USA*

P. Grigolini *

*Center for Nonlinear Science, University of North
Texas, P.O. Box 311427, Denton, Texas 76203-5370, USA*

*Dipartimento di Fisica dell'Università di Pisa
and INFN, Piazza Torricelli 2, 56127 Pisa, Italy*

*Istituto di Biofisica CNR, Area della Ricerca di
Pisa, Via Alfieri 1, San Cataldo 56010 Ghezzano-Pisa, Italy*

B. J. West

*US Army Research Office, Research Triangle Park,
NC 27709, USA*

Abstract

We study a process of anomalous diffusion, based on intermittent velocity fluctuations, and we show that its scaling depends on whether we observe the motion of many independent trajectories or that of a Liouville-like equation driven density. The reason for this discrepancy seems to be that the Liouville-like equation is unable to reproduce the multi-scaling properties emerging from trajectory dynamics. We argue that this conflict between density and trajectory might help us to define the uncertain border between dynamics and thermodynamics, and that between quantum and classical physics as well.

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1 Introduction

In statistical physics we assume two distinct, but equivalent descriptions of the dynamics of physical systems; the trajectories of individual particles and the density function for an ensemble of such trajectories. The dynamics of the trajectories are determined by Hamilton's equations of motion and the evolution of the phase space density is determined by Liouville's equation. The relation between the two pictures is similar to that between the Heisenberg and Schrödinger representations. The word representation clearly indicates that these are just two ways of looking at the same physical phenomenon and it would therefore appear frivolous to question their equivalence. In this paper we do call this equivalence into question. However, we do not elect to formulate a grand theory to establish the difference between the two points of view, this has been done by Petrosky and Prigogine [1,2], but rather we take the more modest approach of establishing an inconsistency based on a simple physical problem.

First let us examine how the connection between trajectories, $x(t)$, and phase space densities, $\sigma(x, t)$, are usually made. A numerical treatment of the phase space density requires, by necessity, a transformation of the Liouville density function $\sigma(x, t)$ into a probability, through the relation

$$p(x_i, t) = \langle \sigma(x_i, t) \rangle \delta x_i \quad (1)$$

where the x -axis is divided into N equal parts indexed by $j = 1, 2, \dots, N$, δx_i is a small phase space interval $(x_i, x_i + \delta x_i)$ and the probability density is normalized to unity at all times

$$\sum_{i=1}^N p(x_i, t) = 1. \quad (2)$$

In statistical mechanics $p(x_i, t)$ is the probability of the system being in the interval $(x_i, x_i + \delta x_i)$ at time t .

As a practical matter, in numerical simulations, the quantity $p(x_i, t)$ is the histogram defined by counting the number of trajectories that lie in the interval $(x_i, x_i + \delta x_i)$ at time t . It is clear that this interval can be made as small as we wish, as long as it remains non-zero in numerical calculations. If we consider a set of initial conditions that produce a sharply peaked Liouville density, the density could either remain peaked as it wanders through phase

* Corresponding author.

Email addresses: mb0015@unt.edu (M. Bologna), grigo@unt.edu (P. Grigolini), westb@aro-emh1.army.mil (B. J. West).

space, or it could spread out, thereby producing the continuous spectrum of $\sigma(x, t)$. There are at least two ways such spreading can occur. The first is by the action of infinitely many degrees of freedom in the system. The second is by trajectory instabilities, that being, chaos produced by nonlinear interactions among the degrees of freedom. The latter situation gives rise to dynamically generated random trajectories, whereas the former does not. The kind of statistics emerging from the former case is the result of an assumption, one that is made regarding the initial states of the system. Thus, statistics in the latter case is a consequence of dynamics whereas in the former case it is the result of an assumption.

It is important to stress that the theoretical concept of probability, or Liouville density, and computational probability are not equivalent. In fact while the theoretical probability could be a very complex function, the computational probability is essentially a relative frequency concept, strongly dependent on the size of the cells that are used in the calculation. The computational probability can be interpreted more as a coarse-grained probability than as a true Liouville density. Consequently, it is not unexpected that the two pictures, that of trajectories and that of densities, at least in principle, might produce different results.

However, we know that trajectories and densities have historically produced the same statistical effects. We know, for example, that when the Markov condition applies, the probabilistic representation, based on trajectories, follows the Central Limit Theorem (CLT). This agrees with the density perspective. In fact, as recently as last year, Lee [3] showed that the adoption of the Liouville approach is compatible, in the long-time limit, with Fick's law, and, consequently, with the tenets of the CLT. In this paper we show that this equivalence is lost when the Generalized CLT (GCLT) of Lévy-Gnedenko [4] applies. In this latter case, the density picture cannot properly reproduce the mechanism of memory erasure necessary for the GCLT to apply. The density representation seems to be more adequate to mimic the relaxation processes, determined by the action of many degrees of freedom, without involving trajectory randomness, and therefore compatible with the existence of an infinite memory.

2 On a time convoluted equation with infinite memory

In this section we derive a single equation of motion for the Liouville density, in two distinct ways. The first is based on the Liouville equation of all the variables, both the diffusing variable x and those responsible for the fluctuations generating the diffusion process under study. The second way is based on the direct integration of the equation of motion for a single trajectory, and serves

essentially the purpose of double checking the generalized diffusion equation resulting from the first method. The first method, identical to that used in an earlier publication[5], is applied imagining that fluctuations are produced by a set of bath variables, and is compatible with the theoretical perspective, on the foundation of statistical mechanics, based on the action of infinitely many degrees of freedom. However, as shown in Appendix, the same result can be obtained by means of trajectory randomness.

2.1 Liouville argument

We consider one of the simplest differential equations

$$\frac{dx(t)}{dt} = \xi(t), \quad (3)$$

where $\xi(t)$ is a two state random process taking the values $\pm W$. If $\phi(x, \xi, t)$ is the phase space distribution function, then the equation of evolution corresponding to the dynamical equation (3) is

$$\frac{\partial}{\partial t} \phi(x, \xi, \mathbf{R}, t) = \left(-\hat{\xi} \frac{\partial}{\partial x} + \hat{\Gamma} \right) \phi(x, \xi, \mathbf{R}, t). \quad (4)$$

We are adopting a quantum-like formalism. Thus, $\hat{\Gamma}$ is an operator characterizing the dynamics of the ξ -process and $\hat{\xi}$ is an operator having the eigenvalues $\pm W$, namely

$$\hat{\xi}|\pm\rangle = \pm W|\pm\rangle. \quad (5)$$

The underlying process generating $\xi(t)$ need not be specified, but one realization of it could be a Hamiltonian system with a set of variables \mathbf{R} . These latter variables can be infinitely many so as to result in the relaxation of the correlation properties of the system.

At equilibrium, the two states $|+\rangle$ and $|-\rangle$ must have the same statistical weight. Thus we assume that the bath equilibrium corresponds to the state

$$|p_0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)\Pi(\mathbf{R}), \quad (6)$$

where $\Pi(\mathbf{R})$ denotes the equilibrium distribution of the variables responsible for the stochastic dynamics of the variable ξ . The state $|p_0\rangle$ is one of the

eigenstates of the operator $\hat{\Gamma}$. In fact, we set

$$\hat{\Gamma}|\mu\rangle = -\Lambda_\mu|\mu\rangle, \quad (7)$$

and $|p_0\rangle = |\mu = 0\rangle$, $\Lambda_0 = 0$. Within this quantum-like formalism the variable ξ , as earlier said, corresponds to the operator $\hat{\xi}$. This operator, applied to the equilibrium state $|p_0\rangle$ yields the excited state

$$|p_1\rangle = \frac{(\hat{\xi}|p_0\rangle)\Pi(\mathbf{R})}{W}. \quad (8)$$

This means that the operator $\hat{\xi}$ does not affect the distribution of \mathbf{R} . It has the effect of making the transitions $|+\rangle + |-\rangle \rightarrow |+\rangle - |-\rangle$ and $|+\rangle - |-\rangle \rightarrow |+\rangle + |-\rangle$, without affecting the other bath variables. The “excited” state $|p_1\rangle$ is not an eigenstate of $\hat{\Gamma}$, but it is a linear combinations of the states $|\mu\rangle$, with $\mu \neq 0$. The operator $\hat{\Gamma}$ applied to the “excited” state $|p_1\rangle$ has the effect of realizing a relaxation by coupling the state $|p_1\rangle$ to infinitely many other eigenstates $|\mu\rangle$. The correlation function $\langle \xi\xi(t) \rangle$, within this quantum-like formalism, reads

$$\langle \xi\xi(t) \rangle = \langle p_0 | \hat{\xi} \exp(\Gamma t) \hat{\xi} | p_0 \rangle. \quad (9)$$

On the basis of the properties of the operators $\hat{\xi}$ and $\hat{\Gamma}$, this correlation function can also be expressed under the form:

$$\langle \xi\xi(t) \rangle = W^2 \sum_{\mu \neq 0} \langle p_1 | \mu \rangle \langle \mu | p_1 \rangle \exp(-\Lambda_\mu t). \quad (10)$$

It is convenient to define

$$\sigma_\mu(x, t) \equiv \langle \mu | \phi(x, \xi, \mathbf{R}, t) \rangle, \quad (11)$$

with $\mu = 0, 1, 2, \dots$. We are interpreting the distribution ϕ of Eq.(4) as a sort of ket vector $|\phi\rangle$. By multiplying Eq. (4) on the left by the states $|\mu\rangle$ we get

$$\frac{\partial}{\partial t} \sigma_0(t) = -W \sum_{\mu \neq 0} a_\mu \frac{\partial}{\partial x} \sigma_\mu(x, t) \quad (12)$$

and, for $\mu > 0$,

$$\frac{\partial}{\partial t} \sigma_\mu(t) = -W \sum_{\mu \neq 0} a_\mu^* \frac{\partial}{\partial x} \sigma_0(x, t) - \Lambda_\mu \sigma_\mu(x, t), \quad (13)$$

with $a_\mu = \langle \mu | \hat{\xi} | p_0 \rangle$.

Let us make the assumption that at $t = 0$ all the σ_μ 's but the one with $\mu = 0$ vanish. This condition is equivalent (see also Appendix) to assuming the spatial distribution to be statistically independent of the “velocity” distribution, and has the nice effect, as we shall see below, of resulting in an equation of motion without an inhomogeneous term. By solving Eq.(13), and replacing the solution into Eq. (12). we get

$$\frac{\partial}{\partial t} \sigma_0(t) = W^2 \sum_{\mu \neq 0} a_\mu \frac{\partial}{\partial x} |a_\mu|^2 \int_0^t dt' \exp[-\Lambda_\mu(t-t')] \frac{\partial^2}{\partial x^2} \sigma_0(x, t'). \quad (14)$$

From now on we shall focus on the reduced density matrix $\sigma_0(x, t)$ and for the sake of simplicity we shall omit the subscript 0. Using Eq.(10) we can rewrite Eq. (14) in the form

$$\frac{\partial}{\partial t} \sigma(x, t) = \int_0^t \langle \xi(t) \xi(t') \rangle \frac{\partial^2 \sigma(x, t')}{\partial x^2} dt'. \quad (15)$$

In the case where the correlation function in (15) is an exponential

$$\langle \xi(t) \xi(t') \rangle = \langle \xi^2 \rangle e^{-\gamma(t-t')}, \quad (16)$$

taking the time derivative of (15) yields

$$\frac{\partial^2 \sigma(x, t)}{\partial t^2} + \gamma \frac{\partial \sigma(x, t)}{\partial t} - \langle \xi^2 \rangle \frac{\partial^2 \sigma(x, t)}{\partial x^2} = 0. \quad (17)$$

This is the celebrated telegrapher's equation, whose phenomenological pedigree originates with Maxwell. His (Maxwell's) argument was to include relaxation into the wave equation and did not require the invocation of microscopic dynamics. However, this use of dissipation was compatible with the action of infinitely many degrees of freedom in the medium supporting the wave motion, and made the Poincaré recurrence times of the dynamics, infinitely long. On the other hand, the case of ordinary statistical mechanics is where we do not find any conflict between the adoption of a density picture and a trajectory picture.

2.2 Trajectory argument

The trajectory for an unforced system rate equation driven by the random function $\xi(t)$, such as (3), is given by

$$x(t) = x(0) + \int_0^t \xi(t') dt'. \quad (18)$$

We again assume that the random driving function can only take on two values, $\pm W$. The fluctuation $\xi(t)$ gets one of these two values for an unpredictable amount of time and in Section II C we shall see that the condition of anomalous diffusion here under study is due to the inverse power nature of the corresponding distribution of sojourn times in each of these two states. In the absence of bias, the odd-order moments of the fluctuations vanish, and using the dichotomous nature of $\xi(t)$ we obtain the factorization result

$$\langle \xi(t_1) \xi(t_2) \cdots \xi(t_{2n-1}) \xi(t_{2n}) \rangle = \langle \xi(t_1) \xi(t_2) \rangle \cdots \langle \xi(t_{2n-1}) \xi(t_{2n}) \rangle. \quad (19)$$

With these conditions on the correlation properties of the random force, introducing the correlation function

$$\Phi_\xi(t_1 - t_2) = \frac{\langle \xi(t_1) \xi(t_2) \rangle}{\langle \xi^2 \rangle}, \quad (20)$$

and using $\langle \xi^2 \rangle = W^2$, it is straight forward to show that the moments of the system response has the convolution form

$$\langle x(t)^{2n} \rangle = (2n)! W^{2n} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{2n-1}} dt_{2n} \times \Phi_\xi(t_1 - t_2) \cdots \Phi_\xi(t_{2n-1} - t_{2n}). \quad (21)$$

Let us consider the Liouville-like equation

$$\frac{\partial \sigma(x, t)}{\partial t} = W^2 \int_0^t \Phi_\xi(t - t') \frac{\partial^2 \sigma(x, t')}{\partial x^2} dt'. \quad (22)$$

This is the same equation as that derived from the quantum-like formalism of Section IIA, Eq. (15). Let us multiply it on the left by x^{2n} and let us integrate

over all phase space yields. After two integrations by parts, we get

$$\frac{d \langle x^{2n}; t \rangle}{dt} = W^2 n(n-1) \int_0^t \Phi_\xi(t-t') \langle x^{2n-2}; t' \rangle dt'. \quad (23)$$

Thus, we can see that following an integration over time we obtain the recursive moment relation

$$\langle x^{2n}; t \rangle = W^2 n(n-1) \int_0^t dt_1 \int_0^{t_1} \Phi_\xi(t_1-t_2) \langle x^{2n-2}; t_2 \rangle dt_2, \quad (24)$$

whose solution, obtained by reinsertion of the equation back into itself, is given by (21). Thus, we have the equivalence between the moments of the dynamical variable and the moments of the phase space variable:

$$\langle x(t)^{2n} \rangle = \langle x^{2n}; t \rangle. \quad (25)$$

The meaning of this result is that Eq. (15) is the proper Liouville-like equation for the dynamic process under study. So, the conflict between trajectory and density, which is the central issue of this paper, cannot be ascribed to the fact that the density equation of motion is questionable. It is not so, the generalized diffusion equation of Eq. (15) generates the same moments as the trajectories. The discrepancy between the two pictures have a deep motivation that we can already try to identify at this level. Paraphrasing Fox[6], we note that the Liouville-like equation of Eq. (15) is not a *bona fide* diffusion equation. This is so because of its irretrievably Non-Markov character that forces us to adopt it always with the same initial condition, the distribution of the coordinate x independent of that of "velocity" ξ . As we shall see, at long times the adoption of the trajectory perspective has, on the contrary, the effect of erasing any form of memory. This is the true reason of the conflict between the two perspectives. The ambiguity resulting from the constraints posed by the moments cannot be invoked. In fact, it is straightforward to show that the moment hierarchy of Eq. (24) fits the Hamburger condition[7] ensuring the uniqueness of the solution of Eq. (15).

2.3 Phase-space equation of motion

The equation of motion for the Liouville density that we obtained using the quantum-like Liouville approach, in a complete accordance with the moment

constraints resulting from the trajectory argument, is of the form

$$\frac{\partial \sigma(x, t)}{\partial t} = \int_0^t \Phi(t - t') \frac{\partial^2 \sigma(x, t')}{\partial x^2} dt' = \int_0^t \Phi(t') \frac{\partial^2 \sigma(x, t - t')}{\partial x^2} dt'. \quad (26)$$

In the case when the correlation function $\Phi(t)$ is integrable, using the last term of the equality of (26), we can easily make the Markov approximation. This is based on replacing $\frac{\partial^2 \sigma(x, t - t')}{\partial x^2}$ with $\frac{\partial^2 \sigma(x, t)}{\partial x^2}$ and in extending the time integration, from 0 to ∞ rather than from 0 to t . Thus we get

$$\frac{\partial \sigma(x, t)}{\partial t} = D \frac{\partial^2 \sigma(x, t)}{\partial x^2}, \quad (27)$$

where the diffusion coefficient D is given by

$$D = W^2 \tau_C \quad (28)$$

and

$$\tau_C = \int_0^\infty dt' \Phi_\xi(t'). \quad (29)$$

Notice that in the Continuous Time Random Walk (CTRW) as used in [8] yields, in the case where the waiting time distribution is exponential, $\psi(t) = a \exp[-at]$, the same evolution for the probability density $p(x, t)$ as that for the phase space distribution $\sigma(x, t)$ resulting from (26). This can be established by noticing that in the case of the dichotomous variable ξ used here, the waiting time distribution is related to the correlation function by the exact relation [9]

$$\Phi_\xi(t) = \frac{1}{\tau_W} \int_t^\infty dt' (t' - t) \psi(t'), \quad (30)$$

where τ_W denotes the mean sojourn time. In the exponential case this sojourn time becomes identical to the correlation time defined by Eq. (29). In other words, since $\Phi_\xi(0) = 1$, in the exponential case $a = \frac{1}{\tau_W}$ and $\tau_C = \tau_W$.

In this paper we study the case where the waiting time distribution $\psi(\tau)$ has the inverse power law form:

$$\psi(\tau) = \frac{(\mu - 1)T^{\mu-1}}{(t + T)^\mu}, \quad (31)$$

where $\mu = \beta + 2$ and T is a parameter determining the length of the laminar region[5]. According to Eq. (30), the corresponding correlation function $\Phi_\xi(t)$ reads

$$\Phi_\xi(t) = \left(\frac{T}{T+t}\right)^\beta. \quad (32)$$

We shall focus our attention on $\beta < 1$. This means that the correlation time τ_C becomes infinite, while the mean waiting time $\tau_W = T/\beta$ remains finite. As pointed out by the authors of Ref. [10], the numerical calculation, based on trajectories, yields a perfect agreement with the predictions of the GCLT at times $t \gg \tau_W$. This means that in this time scale the trajectory treatment yields a distribution that does not keep memory of the initial condition. This is in a striking conflict with the non-Markovian character of Eq. (26), and already affords good reasons to explain the emergence of two distinct solutions from the same equation. Actually, as we shall see, one of these solutions is correct, and it is the unique solution of Eq. (26). The other solution rests on an approximation, necessary to recover the Markov nature of the process described by the GCLT. This is not a genuine solution of Eq. (26): its departure from the exact solution is a measure of the discrepancy between trajectory and density.

It is worth pointing out that the CTRW of Ref.[8] rests on the waiting time distribution $\psi(t)$, whereas the generalized diffusion equation of Eq. (15) is based on the correlation function $\Phi_\xi(t)$. This explains why the former theory is compatible with the Markov character of Lévy diffusion (τ_W is finite) while the latter one is not (τ_C is infinite).

3 On the correct solution to the generalized diffusion equation

We shall investigate the solution to (26) in the case where the correlation time diverges. In the case where there is no correlation time, the determination of the statistical properties of the system depends on whether we analyze the trajectories or the density distribution function. The two "representations" appear to give different results.

3.1 Approximate solution

The closed form solution to (26) depends on the choice of the correlation function in the integrand. We select an inverse power-law correlation function

for the kernel,

$$\Phi(t) = W^2 \frac{T^\beta}{(T+t)^\beta}, \quad (33)$$

with $0 < \beta < 1$, and T is a positive constant. The equation for the density distribution can now be written, with a little adjustment, as

$$\frac{\partial \sigma(x, t)}{\partial t} = W^2 \frac{T^\beta}{(T+t)^\beta} \int_0^t \frac{dt'}{\left(1 - \frac{t'}{T+t}\right)^\beta} \frac{\partial^2 \sigma(x, t')}{\partial x^2}, \quad (34)$$

where we have anticipated that since $t > t'$, we can expand the kernel using the binomial theorem. Retaining the lowest order term in T in the binomial expansion we have

$$\frac{\partial \sigma(x, t)}{\partial t} \approx W^2 \frac{T^\beta}{(T+t)^\beta} \int_0^t \frac{\partial^2 \sigma(x, t')}{\partial x^2} dt', \quad (35)$$

so that defining

$$v(t)^2 \equiv W^2 \frac{T^\beta}{(T+t)^\beta}, \quad (36)$$

we can transform the differential-integral equation (35) into an ordinary partial-differential equation by differentiating this equation in time to obtain

$$\frac{\partial}{\partial t} \left[\frac{1}{v(t)^2} \frac{\partial \sigma(x, t)}{\partial t} \right] = \frac{\partial^2 \sigma(x, t)}{\partial x^2}. \quad (37)$$

Introducing the dimensionless quantities $\tau = 1 + t/T$ and $q = x/WT$, into (37) and taking the Fourier transform with respect to the variable q we arrive at Lommel's equation [11]:

$$\frac{\partial^2 \hat{\sigma}(k, \tau)}{\partial \tau^2} + \frac{\beta}{\tau} \frac{\partial \hat{\sigma}(k, \tau)}{\partial \tau} + \frac{k^2}{\tau^\beta} \hat{\sigma}(k, \tau) = 0, \quad (38)$$

whose solution is expressed in terms of Bessel functions as:

$$\hat{\sigma}(k, \tau) = \tau^{\frac{1-\beta}{2}} \left[a(k) J_\nu \left(\frac{2}{2-\beta} k \tau^{\frac{2-\beta}{2}} \right) + b(\tau) J_{-\nu} \left(\frac{2}{2-\beta} k \tau^{\frac{2-\beta}{2}} \right) \right], \quad (39)$$

where the coefficients $a(k)$ and $b(\tau)$ satisfy the initial conditions:

$$\hat{\sigma}(k, \tau)|_{\tau=1} = 1 \text{ and } \left. \frac{\partial \hat{\sigma}(k, \tau)}{\partial \tau} \right|_{\tau=1} = 0 \quad (40)$$

and $\nu = \frac{1-\beta}{2-\beta}$. After some algebra we obtain

$$a(k) = -\frac{\frac{1-\beta}{2k} J_{-\nu}\left(\frac{2}{2-\beta}k\right) + J'_{-\nu}\left(\frac{2}{2-\beta}k\right)}{\sin \nu \pi} \frac{\pi k}{2-\beta} \quad (41)$$

and

$$b(k) = \frac{\frac{1-\beta}{2k} J_{\nu}\left(\frac{2}{2-\beta}k\right) + J'_{\nu}\left(\frac{2}{2-\beta}k\right)}{\sin \nu \pi} \frac{\pi k}{2-\beta}. \quad (42)$$

Since the argument of the Bessel functions are almost always greater than ν we can adopt the approximation

$$J_{\nu}(z) \approx \sqrt{\frac{2}{\pi z}} \sum_{n=0}^{m-1} \frac{c(n)}{z^n} \cos \left[z - \frac{\pi(2\nu - 2n + 1)}{4} \right], \quad (43)$$

which when inserted into the solution (39) enables us to invert the Fourier transform.

The density distribution resulting from the Fourier inversion of this lowest order solution to the Liouville equation, remembering that q is the Fourier complement to k , is

$$\sigma(x, t) = \frac{T^{\beta/4}}{2(T+t)^{\beta/4}} \delta \left[\frac{|x|}{WT} - \frac{2}{2-\beta} \left(\frac{T^{1-\beta/2}}{(T+t)^{1-\beta/2}} - 1 \right) \right], \quad (44)$$

with the region between the two peaks corresponding to a negligible constant density distribution. What is interesting about this solution is that it has two delta function peaks traveling in opposite directions at a speed which is time dependent. It is a simple matter to check that for early times, $T \gg t$, we have a ballistic propagation front that is characteristic of a system of trajectories with $x \sim \pm Wt$. On the other hand, for late times, $t \gg T$, the distribution has propagation fronts that scale with time as $x \sim \pm t^{1-\beta/2}$, whereas the trajectories themselves would still maintain the ballistic front.

So what have we learned? In the exponential case the trajectory and the density pictures coincide. Now we have also established that for early times,

$T \gg t$, there is no difference in the evolutions of the system between the exponential and inverse power-law correlation functions. This is the reason why the two pictures coincide. However, at late times, when the memory becomes important, the scaling of the trajectory and density pictures appear to be quite different. But this was an approximate solution, what about the exact solution?

3.2 The exact solution

In this section we are interested in the asymptotic behavior of the exact solution to (26). The most direct way to determine these properties is to take the Laplace transform in time and Fourier transform in space to obtain the Fourier-Laplace transform of the Liouville density

$$\hat{\tilde{\sigma}}(k, s) = \frac{1}{s + \tilde{\Phi}(s) k^2}, \quad (45)$$

where we have imposed the initial conditions

$$\sigma(x, t)|_{t=0} = \delta(x) \text{ and } \left. \frac{\partial \sigma(x, t)}{\partial t} \right|_{t=0} = 0. \quad (46)$$

The inverse Fourier transform of (45) yields

$$\tilde{\sigma}(x, s) = \sqrt{\frac{s}{\tilde{\Phi}(s)}} \frac{e^{-|x| \sqrt{\frac{s}{\tilde{\Phi}(s)}}}}{2s}, \quad (47)$$

which we can integrate to obtain

$$\int_{-\infty}^{\infty} \tilde{\sigma}(x, s) dx = \frac{1}{s}, \quad (48)$$

indicating the conservation of normalization over time. To go beyond the formal solution (47) we must specify the correlation function. We assume the inverse power-law form given by (33) so that its Laplace transform becomes

$$\tilde{\Phi}(s) = \frac{\Gamma(1 - \beta) TW^2}{(sT)^{1-\beta}} \left[e^{sT} - E_{\beta-1}^{sT} \right], \quad (49)$$

where the generalized exponential function is defined by [12,13]

$$E_\gamma^x \equiv D_x^\gamma [e^x] = \sum_{n=0}^{\infty} \frac{x^{n-\gamma}}{\Gamma(n+1-\gamma)}. \quad (50)$$

3.2.1 Early time behavior

Let us first consider the behavior of the correlation function at early times. In this domain, $t \rightarrow 0$, we have $s \rightarrow \infty$, so that the generalized exponential becomes

$$E_{\beta-1}^{sT} \approx e^{sT} - \frac{1}{\Gamma(1-\beta)(sT)^\beta}, \quad (51)$$

which when substituted into (49) yields $\tilde{\Phi}(s) \approx W^2/s$ so that the Laplace transform of the early time approximation to the exact solution is

$$\tilde{\sigma}(x, s) \approx \frac{e^{-|x|s/W}}{2W}. \quad (52)$$

The inverse Laplace transform of (52) yields the delta function

$$\sigma(x, t) \approx \frac{1}{2W} \delta\left(t - \frac{|x|}{W}\right). \quad (53)$$

Thus, for times shorter than T , the evolution of the Liouville density consists of two peaks traveling in opposite directions at the same speed, W . Note that this is the same early-time solution obtained in the previous section.

3.2.2 Late time behavior

Now let us consider the asymptotic in time behavior of the exact solution. In the late time domain $t \rightarrow \infty$, we have $s \rightarrow 0$, so examining the behavior of (49) in this domain we have

$$\tilde{\Phi}(s) \approx \frac{\Gamma(1-\beta)TW^2}{(sT)^{1-\beta}} \left[1 - \frac{(sT)^{1-\beta}}{\Gamma(1-\beta)} \right]. \quad (54)$$

Note that as $s \rightarrow 0$ the leading term in this expansion diverges for $\beta < 1$ corresponding to the fact that there is no correlation time for this process.

Inserting this expression for the Laplace transform of the correlation function into (49), keeping only the diverging term, yields

$$\tilde{\sigma}(x, s) \approx \frac{\exp\left[-\frac{|x|s^{1-\beta/2}}{\Gamma(1-\beta)WT^{\beta/2}}\right]}{2\Gamma(1-\beta)W(sT)^{\beta/2}}. \quad (55)$$

The inverse Laplace transform of (55) is

$$\sigma(x, t) \approx \frac{1}{2\langle x \rangle t^{1-\beta/2}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(1-(n+1)(1-\beta/2))} \left(\frac{|x|}{\langle x \rangle t^{1-\beta/2}}\right)^n, \quad (56)$$

where the average of the system variable is

$$\langle x \rangle = WT^{\beta/2}\Gamma(1-\beta), \quad (57)$$

as had been obtained previously [14]. Straight forward dimensional analysis indicates that the space variable scales as $x \sim t^\alpha$, where

$$\alpha = 1 - \beta/2. \quad (58)$$

This scaling is the same scaling as that of the second moment[5,16] and it is different from the Lévy scaling, which is, as we shall see in Section IV, $\alpha = 1/(\beta + 1)$. Thus, in the late time region the exact solution of Eq. (15) departs from the Lévy diffusion, in accordance with the conclusions of the authors of Ref. [15]. It is worth remarking that from a mathematical point of view, according to Ref.[17], the equation of motion admits a solution also for $|x| \gg t^\alpha$. This solution is proved to drop exponentially with $|x|$. We think that the two peaks traveling in the opposite direction of Eq.(44) are a signature of the two ballistic peaks stemming from the numerical calculation based on trajectory dynamics[10,5]. The population beyond these two peaks is rigorously zero. On the basis of this physical suggestion we neglect this contribution to the general solution of Eq. (15). This makes the solution proposed in this paper different from that proposed by the authors of Ref. [15]. However, this is not relevant for the main finding of this paper, the conflict between trajectory and density perspective, since also the solution of the authors of Ref. [15] departs from Lévy statistics. We only note that our choice insures the existence of a unique scaling while the solution of the authors of Ref. [15] does not. To support our conclusion we note that in the asymptotic limit $s \rightarrow 0, k \rightarrow 0$, Eq. (45) yields

$$\hat{\sigma}(k, s) = \frac{1}{s + \text{const } s^{\beta-1}k^2}. \quad (59)$$

The scaling condition $x \sim t^\alpha$ implies $k = s^\alpha$, which plugged into the right hand side term of Eq.(59) makes the left hand side of the same equation proportional to $1/s$ when the scaling condition of Eq. (58) applies. We note that $1/s$ is the Laplace transform of a constant in accordance with the fact that scaling is a reflection of stationarity. For this reason we are inclined to believe that the density perspective yields in the asymptotic limit a unique scaling and that our solution correctly reflects this condition.

4 Lévy scaling

It is clear that the memory effect contained in the correlation function, that is, the memory kernel in (26), implies that the density dynamics are not Markovian. However, as earlier pointed out, the individual trajectories are driven by the waiting time distribution $\psi(\tau)$, and consequently, in accordance with the GCLT, yield the Markov condition under the form of Lévy statistics. Here we discuss how to make Eq. (26) compatible with this Markov condition. This requires the adoption of an unusual form of a Markov approximation. First of all we change the notation from σ to p to stress that we depart from a rigorous treatment in terms of the density σ . Then we identify $p(x, t - t')$ with the change to the probability distribution $p(x)$ occurring when time changes from t' to t , $\Delta p(x, t; t')$. We assume this change to fit the following relation

$$\begin{aligned} \Delta p(x, t; t') &= \frac{1}{2W} \int_{-\infty}^{\infty} \delta \left[t' - \frac{|x - x'|}{W} \right] p(x', t) dx' \\ &- \frac{1}{2W} \int_{-\infty}^{\infty} \delta \left[t' - \frac{|x - x'|}{W} \right] p(x, t) dx'. \end{aligned} \quad (60)$$

The total change is zero, as it can be easily assessed by integrating $\Delta p(x, t; t')$ from $-\infty$ to $+\infty$. This is so because the change is assumed to be determined only by the uniform motion with velocity W . We impose the condition (60) on the form of the Liouville densities in (26). By integrating out the delta functions, and doing some algebra, we obtain the master equation [12]

$$\begin{aligned} \frac{\partial p(x, t)}{\partial t} &= \frac{1}{2W} \int_{-\infty}^{\infty} \left[\frac{\partial^2}{\partial x'^2} \Phi(|x - x'|) \right] p(x', t) dx' \\ &- \frac{1}{2W} \int_{-\infty}^{\infty} \left[\frac{\partial^2}{\partial x'^2} \Phi(|x - x'|) \right] p(x, t) dx'. \end{aligned} \quad (61)$$

Inserting the inverse power-law correlation function into (61), performing the indicated differentiations and taking the limit $kTW \ll 1$ has been shown to yield [12]

$$\frac{\partial p(x, t)}{\partial t} = b \int_{-\infty}^{\infty} \frac{p(x', t) dx'}{|x - x'|^{\beta+2}}, \quad (62)$$

which is the Reisz fractional derivative discovered by Seshadri and West [18] and whose solution is the symmetric Lévy distribution. The approximation of Eq. (60) makes it possible for us to get rid of the time convolution nature of the generalized diffusion equation of Eq.(15). At the same time, this key relation replaces the correlation function $\Phi_{\xi}(t)$ with its second-order derivative, and, consequently, in accordance with Eq. (30), with the waiting time distribution $\psi(\tau)$.

The symmetric Lévy distribution that solves (62) is

$$p(x, t) = \int_{-\infty}^{\infty} e^{ikx} e^{-bt|k|^{\beta+1}} \frac{dk}{2\pi}, \quad (63)$$

which satisfies the scaling relation

$$p(x, t) = \gamma^{\frac{1}{\beta+1}} p\left(\gamma^{\frac{1}{\beta+1}} x, \gamma t\right). \quad (64)$$

From (64) it is clear that the Lévy diffusion process has a scaling, $x \sim t^{\alpha}$, with

$$\alpha = \frac{1}{\beta + 1}. \quad (65)$$

This scaling is consistent with the process generated by the fluctuations of the variable ξ , as proved by the numerical simulation [10]. It is evident that at a given time t , such that $t \gg t_W$, a single trajectory has been sojourning in a given laminar phase a number of times given by

$$N = \frac{t}{t_W}. \quad (66)$$

It is also evident that the position occupied by the diffusing particle at time t is equivalent to the superposition of N variables y_j , $j = 1, 2, \dots, N$, each with the same inverse power-law waiting time distribution and index $\beta + 2$. In fact, the extended time regions, of duration τ_j , where the variable ξ keeps a constant value, either W or $-W$, corresponds to uncorrelated “flights” of

length $|y_j| = W\tau_j$. Thus, the GCLT applies to the superposition of trajectories, resulting in a Lévy process, and we have the scaling with the power-law index given by (64). However, this solution, which agrees with the results of numerical simulation and the predictions of the GCLT, and so with the trajectory perspective, dramatically departs from the unique solution of Eq. (15), illustrated in Section III.

What is the reason for this conflict? The numerical treatment[5,10] shows that there exists a multi-scaling condition. In fact, there is a finite probability that a trajectory, with velocity W , at $t = 0$, maintains this velocity up to a given time t . The number of these trajectories is proportional to the correlation function $\Phi_\xi(t)$, and consequently decays as $1/t^\beta$, with an infinite decay time. These trajectories generates the two side peaks of the broadening distribution, and a ballistic propagation front. This means that the probability distribution does not have a defined scaling, but it is rather the combination of two. The probability distribution, enclosed by the two ballistic peaks is proven numerically[10,5] to have the scaling $\alpha = 1/(\beta + 1)$, namely, the Lévy scaling of Eq.(65). The propagation front, moving ballistically, would yield the scaling $\alpha = 1$. The exact solution of Section III, as we have seen, yields the scaling of Eq. (58), which is a kind of compromise between the ballistic and the Lévy scaling, being smaller than the former and greater than the latter. It seems that the Liouville-like approach is unable to reproduce this multiple scaling condition, and this is probably the reason of conflict between trajectory and density picture.

5 First Consequence: foundation of statistical mechanics

The foundation of statistical mechanics is still the object of debates, and it seems to us that the main conflict is that between the advocates of trajectory randomness and the advocates of the infinitely large number of degrees of freedom, as main ingredient to produce the transition from dynamics to thermodynamics. As an example of the former view we quote Ref. [19]. In this paper, although the importance of using a very large number of degrees of freedom for the foundation of ordinary statistical mechanics is not ruled out, deterministic chaos of classical trajectories is suggested to be the main ingredient for the foundation of statistical mechanics. The authors of this paper[19] derive indeed for temperature an expression more general than that proposed by Boltzmann, and recover the Boltzmann principle in the limiting case of infinite degrees of freedom.

The advocates of infinitely many degrees of freedom, as main ingredient for the foundation of statistical mechanics, are many. The first, as repeatedly stated by Lebowitz, is Boltzmann. In the last few years the traditional point of view of

Boltzmann has been sustained by Lebowitz[20] and by Goldstein [21]. Another aspect of the controversy has to do with the origin itself of entropy production. The former party seems to rest on the impossibility of keeping under control the initial conditions not so much as a consequence of trajectory instability, but much more as a consequence of the infinitely many degrees of the systems that are expected to characterize the systems that at the macroscopic level exhibit thermodynamic properties. In a sense, the conflict between these two distinct perspectives might lead the advocates of the latter party[20,21] to support the derivation of the generalized master equation here under study through the procedure adopted in Section II, with the relaxation process being induced by the action of infinitely many degrees of freedom. The advocates of randomness would probably make the choice of the derivation of Appendix. The two views yield equivalent results in the case of ordinary statistical mechanics. In fact the Fick's law derived in Ref. [3] without involving trajectory randomness is compatible with the CLT accounting for the Gaussian nature of the ordinary diffusion processes. In the case of strange kinetics here under discussion the advocates of randomness, as a source of memory erasure, would probably adopt the Markov approximation of Section IV. This approximation has in fact the attractive property of establishing a perfect agreement with numerical simulation. However, in so doing, the advocates of randomness should acknowledge that the adoption of the generalized Master equation, here under discussion, is not appropriate and that Lévy processes are incompatible with a Liouville-like approach.

The experimental assessment of Lévy statistics might be regarded as a compelling evidence of the existence of random trajectories. These random trajectories, on the other hand, are characterized by a well defined Kolmogorov-Sinai (KS) entropy[22]. In fact, the diffusing trajectories are generated by an intermittent process, and the entropy increase is generated by the random choice of the waiting times of Eq. (31). Since the dynamic realization of Lévy diffusion, with $2 < \mu < 3$ implies the existence of a finite τ_W , the entropy increase per unit of time is fixed and a departure from this ordinary KS condition is expected to take place only for $\mu < 2$, a condition that would yield $\tau_W = \infty$.

6 Second Consequence: Decoherence and spontaneous wave-function collapses

In a recent paper, celebrating 100 years of the quantum[23], Tigmarm and Wheeler emphasize that the de-coherence theory has made obsolete the hypothesis of the wave-function collapses of the founding fathers of quantum mechanics. A classical trajectory is imagined as a succession of dimensionless points, with the particle being located at given time in only one of these positions. This is quite different from a wave function that might imply the

presence of a particle at the same time in different positions, say, two distinct positions. According to de-coherence theory[24] the classical trajectories are recovered because the environment measures, so to speak, the position, and provokes a collapse into one of the two positions. As Tigmak and Wheeler pointed out, this is not a real collapse but only a consequence of the system entanglement with the environment. The reduced density matrix "looks like" the one that would be produced by a real collapse, and while we have the impression of seeing a collapse, actually there has been an entanglement between system and environment, driven by a unitary transformation. This simulacrum of a collapse apparently conflicts with a realistic perspective, but d'Espagnat in a recent paper[25] warns us that the answer to the question "How do we know that there is a stone on the path, or a tree in the courtyard?" must be addressed with caution. He urges us to adopt this approach: "We know that if had a look at the path, to check whether or not we have the impression of seeing a stone, we should actually get the impression in question." It is difficult to support the realistic perspective advocated by Bassi and Ghirardi[26] precisely because wave-function collapses and de-coherence theory produce the same reduced density matrix.

The result of this paper might transform the philosophical debate between d'Espagnat and Bassi and Ghirardi into a real scientific issue. Our arguments are conjectural but plausible. Let us see why. Let us consider Eq. (26). If we move from within a quantum mechanical picture, we have to make the conjecture that the derivation of the classical process of anomalous diffusion must go through this equation. In other words, if the de-coherence program is reliable, and yields any kind of classical diffusion, normal and anomalous, then we expect that it will do it remaining at the level of densities, without ever invoking the concept of trajectory. Of course, the Markovian approximation stemming from Eq.(60) would not be possible and we should therefore give credit to the exact solution of Eq. (26). If, on the contrary, the trajectories exist and are produced by real wave-function collapses, then we expect that the Lévy statistical mechanics might emerge. We would be tempted to say that the experimental assessment of the existence of Lévy processes is a proof of the occurrence of genuine wave-function collapses. It is evident, however, that this would require a more careful derivation from Hamiltonian dynamics, and the experimental assessment of Lévy processes with a microscopic rather than a macroscopic and phenomenological origin.

7 Concluding Remarks

Sections V and VI refer to possible consequences of the results of this paper that are very ambitious. In the final balance of this Section we adopt a much more modest view: we make a short history of the facts that led us to reach the

conclusions illustrated in this paper. A nice dynamic foundation of Lévy processes was given by Zumofen and Klafter[8]. The source of fluctuations used by these authors is very similar to that adopted by us in Appendix. The theory used by them to account for their experimental results is that of CTRW. As already remarked in Section III, this theory is not based on the Liouville-like prescriptions used in this paper, and, it is, in our view compatible with the concept of trajectory. This is why the authors of Ref. [8] found correct and non-contradictory results. The authors of Ref. [5], on the contrary, adopted a Liouville-like approach that led them to establish, for the first time, the generalized diffusion equation here under discussion. However, these authors made use of computer simulation and found that the Markov approximation of Section IV is necessary to establish a satisfactory accordance with the results of numerical simulation. They made also the wrong conjecture that the Markov approximation of Eq. (60) is legitimate from a mathematical as well as from a physical point of view, and that the solution emerging from it is very close to the exact solution, unknown to them. This is the main reason why the later paper of Ref.[27] was fraught by internal contradictions, correctly pointed out by Metzler and Nonnemacher [15] in a subsequent paper. The authors of Ref. [12], having in mind the numerical results of the earlier work[5], used the generalized master equation[28], as a bridge between the Hamiltonian microscopic dynamics and the long-time limit, or macroscopic level, where Lévy statistics show up. The physical arguments are correct and the agreement with the numerical results is remarkable. However, no attention was devoted by these authors[12] to the striking fact that the generalized diffusion equation (15) is incompatible with the Markovian approximation necessary to derive Lévy statistics. We hope that the present paper might serve at least the good purpose of explaining the mathematical and physical reasons behind the contradictory conclusions of the papers of Refs.[5,15,27,12]. We think that this might bear also the significant consequences of establishing the borders between dynamics and thermodynamics (Section IV) and between quantum and classical mechanics (Section V). This will be the object of further research work.

8 APPENDIX: Frobenius-Perron operator for an idealized model of intermittent dynamics

Let us consider the following dynamical system. This is given by a coordinate y moving within the interval $I = [0, 2]$ with the equation of motion

$$\frac{dy}{dt} = -\frac{dV(y)}{dy} = -W(y). \quad (\text{A-1})$$

This is a form of overdamped dynamics within the "potential" $V(y)$, with the function $W(y)$ defined by

$$W(y) = \text{sign}(y - 1)\lambda|y - 1|^z, \quad (\text{A-2})$$

where $\text{sign}(x)$ denotes the sign of x . The particle with coordinate y moves within a potential with the minimum located at $y = 1$. Thus, if the initial condition of the particle is $y(0) > 1$, the particle moves from the right to the left towards the potential minimum. If the initial condition is $y(0) < 1$, then the motion of the particle towards the potential minimum takes place from the left to the right. When the particle reaches the potential bottom is injected to an initial condition, different from $y = 1$, chosen in a random manner. We thus realize a mixture of randomness and slow deterministic dynamics. The left and the right portions of the potential $V(y)$ correspond to the laminar regions of turbulent dynamics, while randomness is concentrated at $y = 1$. It is straightforward to prove that the waiting time distribution in any of the two laminar regions is given by

$$\psi(\tau) = \frac{(\mu - 1)T^{\mu-1}}{(T + \tau)^\mu}, \quad (\text{A-3})$$

where $\mu = z/(z - 1)$ and $T = (\mu - 1)/\lambda$. Eq.(3) must be written now as

$$\frac{dx}{dt} = \xi(y(t)), \quad (\text{A-4})$$

with $\xi(y) = W$ if $1 < y \leq 2$, and $\xi(y) = -W$ if $0 < y \leq 1$. The hamiltonian formulation corresponding to this kind of sporadic randomness with an inverse power law distribution has been discussed in detail by Zaslavsky[29]. Unfortunately, this Hamiltonian treatment would make the calculations more complicated. We think that the current treatment, although not Hamiltonian, shares the main dynamic properties of Zaslavsky's dynamics. In this idealization the size of the chaotic region is reduced to $y = 1$, with a virtually instantaneous back injection into the laminar region. In the Hamiltonian models of Zaslavsky, on the contrary, the particle spends some time in the chaotic region, with no significant consequences on the asymptotic time properties, though, since these are dominated by the laminar motion, due to the inverse power law nature of the waiting time distribution.

In this case the Liouville-like equation for the whole phase space (x, y) reads

$$\frac{\partial}{\partial t}\phi(x, y, t) = \hat{L}_T\phi(x, y, t), \quad (\text{A-5})$$

where the Frobenius-Perron operator of the whole system, \hat{L}_T , is given by

$$\hat{L}_T \equiv -\xi(y)\frac{\partial}{\partial x} + \hat{L}_B. \quad (\text{A-6})$$

The first term on the right hand side of this equation represents the interaction between the diffusing variable x and the fluctuation ξ driven by the intermittent dynamics of the variable y . The Frobenius-Perron operator corresponding to this "bath" dynamics is given by

$$\hat{L}_B[\cdot] \equiv \frac{\partial}{\partial y}V(y)[\cdot] + \frac{1}{\tau_{random}} \int_0^2 dy \delta(y-1)[\cdot]. \quad (\text{A-7})$$

We assign to the back injection a finite time τ_{random} , whose actual value is not important for the present discussion, provided that it is assumed to be very short compared to the mean waiting time τ_W . The second term on the right hand side of Eq. (A-7) becomes active only if the probability distribution does not vanish for $y = 1$. In that case it contributes an increase of the population at any value $y \neq 1$, with uniform probability. If it vanishes, the time evolution of the distribution density is not affected by the back injection. When the condition of equilibrium are reached, and the distribution of y is at equilibrium the process of back injection becomes time independent[22]. Using the method of analysis developed in Ref. [22], it is possible to find the bath equilibrium distribution $\eta(y)$, namely, the distribution fulfilling the condition

$$\hat{L}_B\eta(y) = 0. \quad (\text{A-8})$$

We are now equipped to adopt the Zwanzig projection method[30]. The projection operator P works according to the following prescription

$$P\phi(x, y, t) = \sigma(x, t)\eta(y). \quad (\text{A-9})$$

Let us assume the factorized initial condition: $\phi(x, 0) = \sigma(x, 0)\eta(y)$. The Zwanzig projection method yields the following reduced equation of motion

$$\frac{\partial}{\partial t}\sigma(x, t) = \frac{1}{\eta(y)} \int_0^t P\hat{L}_T e^{Q\hat{L}_T(t-t')} Q\hat{L}_T P\phi(x, y, t') dt', \quad (\text{A-10})$$

where $Q \equiv 1 - P$. By exploiting the dichotomous nature of the variable ξ , it is straightforward to prove that Eq.(A-10) yields Eq.(15). This confirms that this generalized diffusion equation is the proper representation of the dynamic process under study. The conflict between trajectory and density perspective

cannot be ascribed to a questionable use of the rules currently adopted to establish the connection between density and trajectory perspective.

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